Bosonization of dimerized Hubbard chains

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The role of Klein factors is investigated for the bosonized Hamiltonian of the dimerized Hubbard model. Contrary to previous approaches we take into account their number changing property, i.e. we do not replace them by Majorana fermions. We show how to treat Klein factors in the framework of the self-consistent harmonic approximation, both for finite systems and in the thermodynamic limit.

1 Introduction

The foundations of bosonization were laid more than 50 years ago in a seminal paper by Tomonaga [1]. During the following decades the method was worked out and successfully applied to one-dimensional electron and spin systems [2, 3, 4]. Despite its long history there are still some subtle points in the bosonization formalism which are not taken into consideration in the majority of the literature. One of these is the proper treatment of the so-called Klein factors which have to be introduced in order to preserve the anticommuting property of the fermionic fields during the bosonization procedure. The role of the Klein factors deserves particular attention when nonlinear perturbations arising e.g. from impurity scattering or lattice modulations are to be considered in finite systems.

In this paper we demonstrate how to handle the Klein factors in a systematic way, both in the thermodynamic limit and for finite systems. As a prototypical model we study the one-dimensional dimerized Hubbard model where the hopping is periodically modulated due to the Peierls distortion of the lattice. We extend the self-consistent harmonic approximation [5, 6, 7] by treating bosonic fields and Klein factors on equal footing [8]. As an application we use the formalism to calculate spin and charge gaps of this model.

2 Bosonization and Klein factors

We consider the dimerized Hubbard model

$$H = -t \sum_{i,\sigma} (1 + (-1)^i u)(c_{i\sigma}^+ c_{i+1,\sigma} + c_{i+1,\sigma}^+ c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

which differs from the ordinary one-dimensional Hubbard model by a periodic modulation of the hopping described by the dimerization parameter u. This modulation is relevant in one dimension due to the coupling between the lattice and the electronic degrees of freedom. A finite u corresponds to a periodic lattice distortion known as Peierls instability. We study the case of half-filling, and have chosen the modulation accordingly to be of the form $(-1)^i u$. The quantity u is considered to be a parameter of the model. $c_{i\sigma}^+$ creates an electron with spin direction $\sigma = \uparrow, \downarrow$ at site i, and t and U are the hopping matrix element and the on-site Hubbard interaction, respectively.

In the following we list the main steps which have to be performed in order to bosonize the Hamiltonian (1). For more details we refer the reader to the reviews [3, 4, 6]. First we represent H in momentum space:

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$$H = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + tu \sum_{k,\sigma} (e^{ik} c_{k\sigma}^+ c_{k+\pi,\sigma} + \text{h.c.}) + \frac{U}{N} \sum_{k,k',q} c_{k+q,\uparrow}^+ c_{k\uparrow} c_{k'-q,\downarrow}^+ c_{k'\downarrow} \tag{2}$$

where $\epsilon_k = -2t \cos k$, and N is the number of lattice sites. We linearize the spectrum around the two Fermi points $\pm k_F$, $k_F = \pi/2$, and introduce left and right moving fermions labeled by L and R, respectively. This allows us to sort the various scattering processes according to their initial and final states ("g-ology"). Then we define bosonic operators $b_{q\alpha}^+$ which are related to fermionic particle-hole excitations via [$\Psi_{L/R\sigma}(k) = c_{\mp(k_F+k),\sigma}$ etc.; $c_{k\sigma}$, $c_{k\sigma}^+$ are the standard Fermion operators]

$$b_{q\alpha}^+ = -\frac{i}{\sqrt{n_q}} \sum_k \Psi_\alpha^+(k+q)\Psi_\alpha(k) \quad (q > 0) \tag{3}$$

where $q = (2\pi/N)n_q$ and $\alpha = R\uparrow, L\uparrow, R\downarrow, L\downarrow$. Returning to real space we define the bosonic fields

$$\varphi_{L\sigma}(x) = \sum_{q>0} \frac{1}{\sqrt{n_q}} b_{qL\sigma} e^{-iqx-aq/2} \;,\; \varphi_{R\sigma}(x) = -\sum_{q>0} \frac{1}{\sqrt{n_q}} b_{qR\sigma} e^{iqx-aq/2} \;,\; a \to 0 \tag{4}$$

which are related to the fermionic field operators via the bosonization identities

$$\Psi_{L\sigma}(x) = \frac{1}{\sqrt{L}} F_{L\sigma} e^{-i\varphi_{L\sigma}^+(x)} e^{-i\varphi_{L\sigma}(x)} e^{-2\pi i N_{L\sigma} x/L} \tag{5}$$

$$= \frac{1}{\sqrt{2\pi a}} F_{L\sigma} e^{-i(\varphi_{L\sigma}^+(x)+\varphi_{L\sigma}(x))} e^{-2\pi i N_{L\sigma} x/L} \tag{6}$$

$$\Psi_{R\sigma}(x) = \frac{1}{\sqrt{2\pi a}} F_{R\sigma} e^{+i(\varphi_{R\sigma}^+(x)+\varphi_{R\sigma}(x))} e^{+2\pi i N_{R\sigma} x/L} \tag{7}$$

where N_α counts the particle number with respect to the filled Fermi sea, and L is the length of the system.[1] The Klein factors F_α^+ (F_α) are unitary operators that commute with the bosonic fields. They change the number of the fermion species α by ± 1, a change which cannot be achieved by any combination of the bosonic field operators. In order to ensure the correct anticommutation relations for $\Psi_\alpha(x)$, the Klein factors have to fulfill the following relations:

$$\{F_\alpha, F_\beta\} = \{F_\alpha^+, F_\beta^+\} = 0, \qquad \{F_\alpha^+, F_\beta\} = 2\delta_{\alpha\beta}, \qquad [N_\alpha, F_\beta] = -\delta_{\alpha\beta} F_\beta \;. \tag{8}$$

Here $[.,.]$ denotes the commutator, and $\{.,.\}$ the anticommutator. In a last step one combines φ_α and φ_α^+ to new fields $\phi_{c,s}$ and $\theta_{c,s}$,

$$\phi_{c,s} = \frac{1}{2\sqrt{2}} (\varphi_{L\uparrow} \pm \varphi_{L\downarrow} + \varphi_{R\uparrow} \pm \varphi_{R\downarrow} + \text{h.c.}) \tag{9}$$

$$\theta_{c,s} = \frac{1}{2\sqrt{2}} (\varphi_{L\uparrow} \pm \varphi_{L\downarrow} - \varphi_{R\uparrow} \mp \varphi_{R\downarrow} + \text{h.c.}) \tag{10}$$

and introduces $N_{c,s} = N_\uparrow \pm N_\downarrow$ and $J_{c,s} = J_\uparrow \pm J_\downarrow$ where $N_\sigma = N_{L\sigma} + N_{R\sigma}$ and $J_\sigma = N_{L\sigma} - N_{R\sigma}$. Combining everything we obtain

$$H = H_0 + H_1 + H_2 + H_3 \tag{11}$$

where H_0 is the Luttinger Hamiltonian:

$$H_0 = \sum_{\alpha=c,s} \int_0^L \frac{dx}{2\pi} : \left\{ \frac{v_\alpha}{g_\alpha} (\partial_x \phi_\alpha)^2 + v_\alpha g_\alpha (\partial_x \theta_\alpha)^2 \right\} : + \frac{\pi}{4L} \sum_{\alpha=c,s} \left\{ \frac{v_\alpha}{g_\alpha} N_\alpha^2 + v_\alpha g_\alpha J_\alpha^2 \right\} \;; \tag{12}$$

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[1] We have chosen the lattice constant to be unity, i.e. $L = N$. Nevertheless we retain L and N for easy reference.

H_1 the Umklapp contribution:

$$H_1 = \tilde{U} \int_0^L dx \, \{F_{R\uparrow}^+ F_{R\downarrow}^+ F_{L\downarrow} F_{L\uparrow} \mathrm{e}^{-i2\sqrt{2}\phi_c} + \mathrm{h.c.}\} \,, \qquad \tilde{U} = \frac{UL}{(2\pi a)^2 N} \,; \tag{13}$$

H_2 the backscattering contribution:

$$H_2 = \tilde{U} \int_0^L dx \, \{F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} \mathrm{e}^{-i2\sqrt{2}\phi_s} + \mathrm{h.c.}\} \,; \tag{14}$$

and H_3 the dimerization contribution ($\tilde{u} = tu/\pi a$):

$$H_3 = \tilde{u} \int_0^L dx \, \{i F_{R\uparrow}^+ F_{L\uparrow} \mathrm{e}^{-i\sqrt{2}(\phi_c+\phi_s)} + i F_{R\downarrow}^+ F_{L\downarrow} \mathrm{e}^{-i\sqrt{2}(\phi_c-\phi_s)} + \mathrm{h.c.}\} \,. \tag{15}$$

In Eqs. (13) – (15) we have used $N_c = N_s = 0$ at half filling. The parameter a is a short-distance cutoff of the order of the lattice spacing, i.e. of order one. The Luttinger parameters $g_{c,s}$ and the charge and spin velocities $v_{c,s}$ can either be calculated perturbatively or from the Bethe ansatz solution of the Hubbard model [9, 10]. In the following we focus on the role of the Klein factors. In the literature it is common practice either to ignore them or to replace them by Majorana fermions [4, 11]. It is argued that the latter approach – which neglects the number changing property of the Klein factors – should be justified in the thermodynamic limit. In the following we aim to present a more rigorous approach. Due to the conservation of charge and spin all combinations of Klein factors appearing in the Hamiltonian (11) can be expressed in terms of the operators $A_\uparrow = F_{R\uparrow}^+ F_{L\uparrow}$ and $A_\downarrow = F_{R\downarrow}^+ F_{L\downarrow}$ plus their hermitean conjugates. In particular, the four-fermion terms arising from Umklapp and backscattering read

$$F_{R\uparrow}^+ F_{R\downarrow}^+ F_{L\downarrow} F_{L\uparrow} = F_{R\uparrow}^+ F_{L\uparrow} F_{R\downarrow}^+ F_{L\downarrow} = A_\uparrow A_\downarrow \,, \tag{16}$$

$$F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} = F_{R\uparrow}^+ F_{L\uparrow} F_{L\downarrow}^+ F_{R\downarrow} = A_\uparrow A_\downarrow^+ \,. \tag{17}$$

Since the Klein factors are unitary, $F_\alpha^+ F_\alpha = F_\alpha F_\alpha^+ = 1$, it is easy to show that

$$[A_\uparrow, A_\uparrow^+] = [A_\downarrow, A_\downarrow^+] = 0 \,, \tag{18}$$

and we may choose a basis where A_σ and A_σ^+ are both diagonal. From $A_\uparrow^+ A_\uparrow = A_\downarrow^+ A_\downarrow = 1$ one concludes that the eigenvalues of A_σ are pure phase factors, i.e.

$$A_\uparrow |k_\uparrow, k_\downarrow\rangle = \mathrm{e}^{ik_\uparrow} |k_\uparrow, k_\downarrow\rangle \qquad A_\uparrow^+ |k_\uparrow, k_\downarrow\rangle = \mathrm{e}^{-ik_\uparrow} |k_\uparrow, k_\downarrow\rangle \tag{19}$$

$$A_\downarrow |k_\uparrow, k_\downarrow\rangle = \mathrm{e}^{ik_\downarrow} |k_\uparrow, k_\downarrow\rangle \qquad A_\downarrow^+ |k_\uparrow, k_\downarrow\rangle = \mathrm{e}^{-ik_\downarrow} |k_\uparrow, k_\downarrow\rangle \tag{20}$$

with $0 \leq k_\sigma < 2\pi$. The terms $\sim J_{c,s}^2$ appearing in H_0 do not commute with the Klein factors; however it appears reasonable to neglect them in the thermodynamic limit $L \to \infty$. We will come back to this question in Sec. 4. We thus replace the Klein factors in H_1, H_2 and H_3 by their eigenvalues, and obtain

$$H_1 = \tilde{U} \int_0^L dx \, \{\mathrm{e}^{i(k_\uparrow+k_\downarrow)} \mathrm{e}^{-i2\sqrt{2}\phi_c} + \mathrm{h.c.}\} \tag{21}$$

$$H_2 = \tilde{U} \int_0^L dx \, \{\mathrm{e}^{i(k_\uparrow-k_\downarrow)} \mathrm{e}^{-i2\sqrt{2}\phi_s} + \mathrm{h.c.}\} \tag{22}$$

$$H_3 = \tilde{u} \int_0^L dx \, \{i\mathrm{e}^{ik_\uparrow} \mathrm{e}^{-i\sqrt{2}(\phi_c+\phi_s)} + i\mathrm{e}^{ik_\downarrow} \mathrm{e}^{-i\sqrt{2}(\phi_c-\phi_s)} + \mathrm{h.c.}\} \,. \tag{23}$$

As a result the Hamiltonian of the dimerized Hubbard model separates into different sectors of purely bosonic Hamiltonians which are labeled by $k_\uparrow$ and $k_\downarrow$. Note that when replacing Klein factors by Majorana fermions [4] one obtains only the eigenvalues $\pm i$ for the two-fermion terms and ± 1 for the four-fermion terms, i.e. continuity is lost. Shifting the field operators according to $\phi_{c,s} \to \phi_{c,s} + (k_\uparrow \pm k_\downarrow)/2\sqrt{2}$, the phase factors can be absorbed, with the result

$$H = H_0 + 2\tilde{U} \int_0^L dx \, (\cos 2\sqrt{2}\phi_c + \cos 2\sqrt{2}\phi_s) + 4\tilde{u} \int_0^L dx \, \sin\sqrt{2}\phi_c \cos\sqrt{2}\phi_s \ . \tag{24}$$

In this sine-Gordon-like Hamiltonian the operator constraint $[\phi_{c,s}]_{q=0} = 0$, see Eq. (4), has to be replaced by

$$\int_0^L dx \, \phi_{c,s} = \frac{L}{2\sqrt{2}}(k_\uparrow \pm k_\downarrow) \ . \tag{25}$$

3   The self-consistent harmonic approximation

In order to study the charge and spin gaps in the dimerized Hubbard model we use the self-consistent harmonic approximation (SCHA) in which the exponentials of field operators appearing in (21) – (23) are replaced by quadratic forms. We introduce the trial Hamiltonian

$$H_{\rm tr} = \sum_{\alpha=c,s} \int_0^L \frac{dx}{2\pi} \left\{ \frac{v_\alpha}{g_\alpha}(\partial_x \phi_\alpha)^2 + v_\alpha g_\alpha (\partial_x \theta_\alpha)^2 + \frac{\Delta_\alpha^2}{v_\alpha g_\alpha}\phi_\alpha^2 \right\} \tag{26}$$

which provides us with a variational estimate for the ground state energy

$$\tilde{E} = \langle H_0 \rangle_{\rm tr} + \langle H_1 \rangle_{\rm tr} + \langle H_2 \rangle_{\rm tr} + \langle H_3 \rangle_{\rm tr} \ , \tag{27}$$

$$\frac{\tilde{E}}{L} = \frac{E_{\rm tr}}{L} - \sum_{\alpha=c,s} \frac{\Delta_\alpha^2 \langle \phi_\alpha^2 \rangle_{\rm tr}}{2\pi v_\alpha g_\alpha} + E(k_\uparrow, k_\downarrow) \ . \tag{28}$$

Here the expectation value is with respect to the ground state of $H_{\rm tr}$, $E_{\rm tr}$ is its ground state energy, and

$$E(k_\uparrow, k_\downarrow) = 2B_1 \cos(k_\uparrow + k_\downarrow) + 2B_2 \cos(k_\uparrow - k_\downarrow) - 2B(\sin k_\uparrow + \sin k_\downarrow) \tag{29}$$

with

$$B_1 = \tilde{U} \, {\rm e}^{-4\langle \phi_c^2 \rangle_{\rm tr}}, \quad B_2 = \tilde{U} \, {\rm e}^{-4\langle \phi_s^2 \rangle_{\rm tr}}, \quad B = \tilde{u} \, {\rm e}^{-\langle \phi_c^2 \rangle_{\rm tr}}{\rm e}^{-\langle \phi_s^2 \rangle_{\rm tr}} \ . \tag{30}$$

Minimizing $\tilde{E}$ with respect to Δ_c and Δ_s yields the gap equations

$$\frac{\Delta_c^2}{2\pi v_c g_c} = -4B_1 \frac{\partial E_0}{\partial B_1} - B \frac{\partial E_0}{\partial B} \tag{31}$$

$$\frac{\Delta_s^2}{2\pi v_s g_s} = -4B_2 \frac{\partial E_0}{\partial B_2} - B \frac{\partial E_0}{\partial B} \tag{32}$$

where E_0 is the minimum of $E(k_\uparrow, k_\downarrow)$ (see Table 1).   In order to solve these equations analytically we consider the case $U > 0$ where $g_s = 1$ and $g_c < 1$, and restrict ourselves to the limit of small dimerization u. Since $H_{\rm tr}$ is quadratic in the bosonic fields it is straightforward to calculate

$$\langle \phi_c^2 \rangle_{\rm tr} = \frac{g_c}{2} \ln \frac{\Delta_0}{\Delta_c} \tag{33}$$

$$\langle \phi_s^2 \rangle_{\rm tr} = \frac{g_s}{2} \ln \frac{\Delta_0}{\Delta_s} \tag{34}$$

range	$k_\uparrow$	$k_\downarrow$	$E_0(B_1, B_2, B)$
$0 < B < 2B_2$	$\arcsin \frac{B}{2B_2}$	$\pi - \arcsin \frac{B}{2B_2}$	$-2B_1 - 2B_2 - \frac{B^2}{B_2}$
$2B_2 < B$	$\frac{\pi}{2}$	$\frac{\pi}{2}$	$-4B - 2B_1 + 2B_2$

Table 1 Minimum E_0 of $E(k_\uparrow, k_\downarrow)$ – see Eq. (29) – which is used in the gap equations (31) and (32). The first line is applicable for $u = 0$ (Hubbard model without dimerization) whereas the second line applies for $u > 0$.

where Δ_0 is a cutoff-dependent energy scale of the order of the bandwidth, and $\Delta_{c,s} < \Delta_0$ is assumed. For nonzero dimerization $u > 0$ the solutions of the gap equations lie in the range $B > 2B_2$; thus the second line of Table 1 with $\partial E_0/\partial B_1 = -2$, $\partial E_0/\partial B_2 = 2$ and $\partial E_0/\partial B = -4$ has to be used in Eqs. (31), (32). For $u \to 0$ the spin gap vanishes while the charge gap approaches a constant according to [12]

$$\Delta_c(u) - \Delta_c(0) \quad \propto \quad u^{4/3} \tag{35}$$

$$\Delta_s(u) \quad \propto \quad u^{2/3} \tag{36}$$

with cutoff-dependent prefactors. The exponent $2/3$ that characterizes the spin gap is in accordance with the corresponding exponent of the dimerized antiferromagnetic Heisenberg chain up to a logarithmic correction in the prefactor [13, 14]. Since the Heisenberg model corresponds to the $U \to \infty$ limit of the half-filled Hubbard model, this indicates that as far as the exponent is concerned the SCHA result (36) is exact and persists even in the strong-coupling regime $U/t \gg 1$. For $u > u_{\mathrm{co}}$ the behavior of the gaps is changed to [15]

$$\Delta_c(u) \approx \Delta_s(u) \quad \propto \quad u^{2/(3-g_c)} \tag{37}$$

where the crossover value u_{co} is defined by $\Delta_s(u_{\mathrm{co}}) = \Delta_c(0)$. In Fig. 1 we show $\Delta_c(u) - \Delta_c(0)$ and $\Delta_s(u)$ as a function of u for $U/t = 2$ as obtained from the numerical solution of the gap equations. For comparison, the analytical results (35) and (36) are also given.

4 Finite systems

For a finite system of length L it is not possible to simply replace the Klein factors by their eigenvalues since the terms $\sim J_{s,c}^2$ in the Luttinger Hamiltonian (12) do not commute with the $F's$. However one may decouple the Klein factors from the bosonic fields using a variational ansatz. To this end we introduce the "Klein Hamiltonian"

$$
\begin{aligned}
H_{\mathrm{tr}}^B &= iB(F_{R\uparrow}^+ F_{L\uparrow} + F_{R\downarrow}^+ F_{L\downarrow}) + B_1 F_{R\uparrow}^+ F_{R\downarrow}^+ F_{L\downarrow} F_{L\uparrow} + B_2 F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} + \mathrm{h.c.} \\
&\quad + \frac{\pi}{4L}(v_c g_c J_c^2 + v_s g_s J_s^2)
\end{aligned} \tag{38}
$$

where B_1, B_2 and B are variational parameters to be determined self-consistently. H_{tr}^B is of the form of a tight-binding Hamiltonian for a particle moving on a $2d$ lattice in a harmonic potential. A class of similar Hamiltonians for general potentials in $1d$ has been studied in [16]. The choice of the trial Hamiltonian is equivalent to a decoupling of the non-linearities according to

$$
\begin{aligned}
&F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} \mathrm{e}^{-i2\sqrt{2}\phi_s} \to \\
&\langle F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} \rangle_{\mathrm{tr}} \mathrm{e}^{-i2\sqrt{2}\phi_s} + F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow} \langle \mathrm{e}^{-i2\sqrt{2}\phi_s} \rangle_{\mathrm{tr}} ,
\end{aligned} \tag{39}
$$

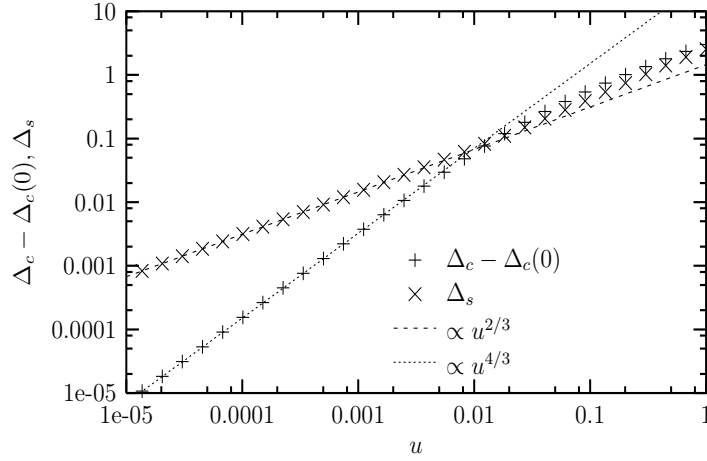**Fig. 1** Charge gap Δ_c and spin gap Δ_s (in units of t) of the dimerized Hubbard model for $U/t = 2$ obtained within the SCHA. [We used $v_{c,s} = v_F\sqrt{1 \pm U/\pi v_F}$, $g_s = 1$, and $g_c = 1/\sqrt{1 + U/\pi v_F}$; note that $v_F = 2t$]. The straight lines are the analytic results (35) and (36) valid for $u < u_{co}$. Note that $\Delta_c(0)$ is subtracted from the charge gap in order to highlight the power law behavior.

and analogously for the Umklapp and dimerization term. This means that instead of replacing the products of Klein factors by their *eigenvalues* as in the thermodynamic limit, we now have to replace them by their *expectation values* with respect to the ground state of H_{tr}^B. In both cases one ends up with a sine-Gordon type model like the one explicitly given in Eq. (24). It is conceivable that for a finite-size system the eigenvalues are not identical to the expectation values, i.e. different sine-Gordon models arise.

The question is then whether identical sine-Gordon models arise at least in the thermodynamic limit. We can answer this question within the framework of the SCHA. Here the introduction of the "Klein Hamiltonian" amounts to replacing the quantity $E_0(B_1, B_2, B)$ which enters the gap equations (and which is explicitly given in Table 1) by the ground state energy of H_{tr}^B. Apart from this modification Eqs. (30) – (32) remain unchanged. Consider first a system with both a spin and a charge gap. For large systems the parameters B, B_1, and B_2 become size-independent, with the consequence that the kinetic energy in H_{tr}^B dominates the confining potential. The ground state energy of H_{tr}^B is then given by the minimum of $E(k_\uparrow, k_\downarrow)$, see Eq. (29), and expectation values of the Klein factors are equal to their eigenvalues.

In the absence of dimerization, i.e. for the "pure" Hubbard model, we encounter a different situation since the spin gap vanishes. For large system size one finds $B = 0$, $B_1 = \text{const}$, and $B_2 \propto \tilde{U}(a/L)^2$. Thus the confining potential in the spin sector dominates the corresponding kinetic energy (proportional to B_2) in the thermodynamic limit. Hence the ground state of H_{tr}^B is the eigenstate of the current operator with $J_s = 0$, and the expectation value of the operator $F_{R\uparrow}^+ F_{L\downarrow}^+ F_{R\downarrow} F_{L\uparrow}$ in this state is zero, in contrast to the eigenvalues which are $\exp(ik_\uparrow - ik_\downarrow)$, see Eqs. (16) – (20).

5   Conclusions

We studied the role of Klein factors for the bosonized Hamiltonian of the dimerized Hubbard model. Since the Klein operators do not commute with the total spin and charge currents $J_{c,s}$ they cannot acquire a definite value at the same time as the current operators.

The ground state of the gapped system is a superposition of many spin and charge states. In this situation it is justified to choose a fixed phase for the Klein operators. The bosonized Hamiltonian is then the conventional sine-Gordon-like Hamiltonian, cf. Eq. (24). In an ungapped system where the non-linearities

introduced by backscattering are (marginally) irrelevant operators, the ground state has a well defined current. In this case the phase of the Klein operators is undetermined and Eq. (24) has no justification.

We have extended the self-consistent harmonic approximation in such a way that Klein factors can be handled systematically, and we worked out the theory for the Hubbard model. In a previous paper [8] we applied the SCHA to spinless fermions with nearest-neighbor interaction and dimerization, and studied in detail finite-size effects. In the spinless case the Klein Hamiltonian H_{tr}^{B} can be mapped onto a Mathieu equation which can be solved analytically in certain limits. It turns out that finite-size corrections to the gap equation are not important as long as the dimerization gap is larger than the finite-size gap. In addition, the finite-size formalism allows to calculate the size-dependence of the Drude weight in the gapped regime [8].

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